Sample name: **M09_octanol** Experiment start time: **3/6/2018 3:40:58 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-06007** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**

pH-metric Result

logP (XH +)   0.91   ±0.07 (n=50)
logP (neutral X)   3.05   ±0.02 (n=50)

18C-06007 Points 1 to 23

M09_octanol concentration factor 1.046
Carbonate 0.0318 mM
Acidity error 0.09711 mM

18C-06007 Points 24 to 50

M09_octanol concentration factor 0.952
Carbonate 0.0262 mM
Acidity error 0.24086 mM

18C-06007 Points 51 to 74

M09_octanol concentration factor 0.937
Carbonate 0.0860 mM
Acidity error 0.30528 mM

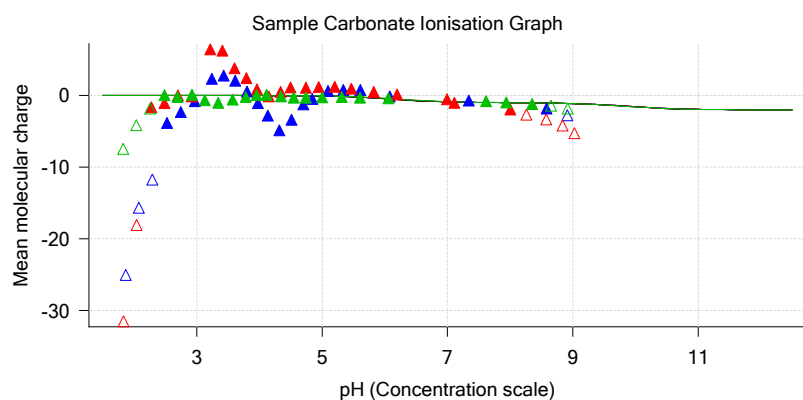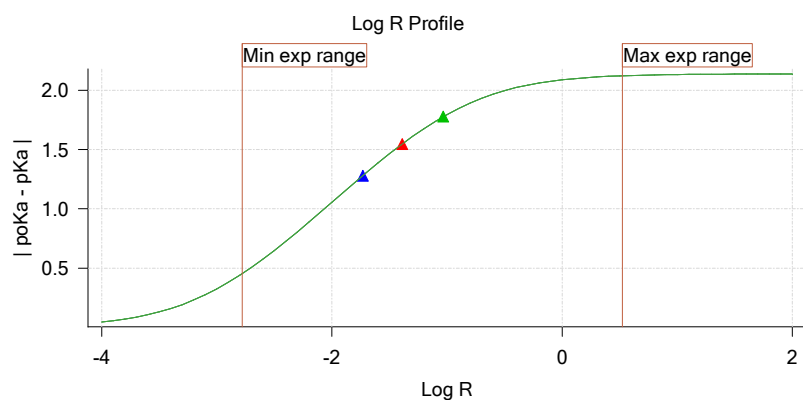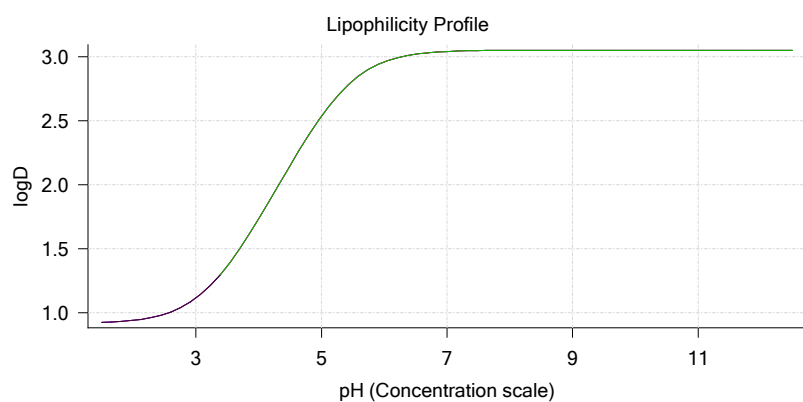## Warnings and errors
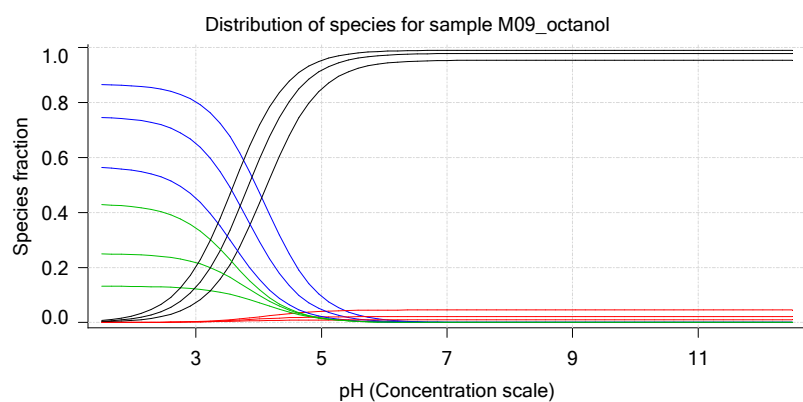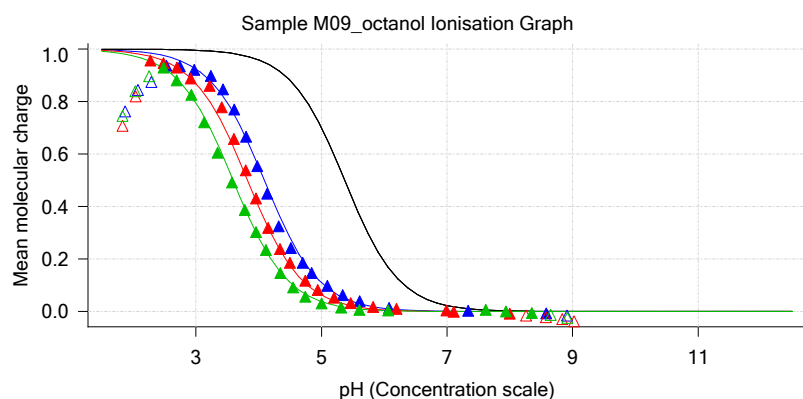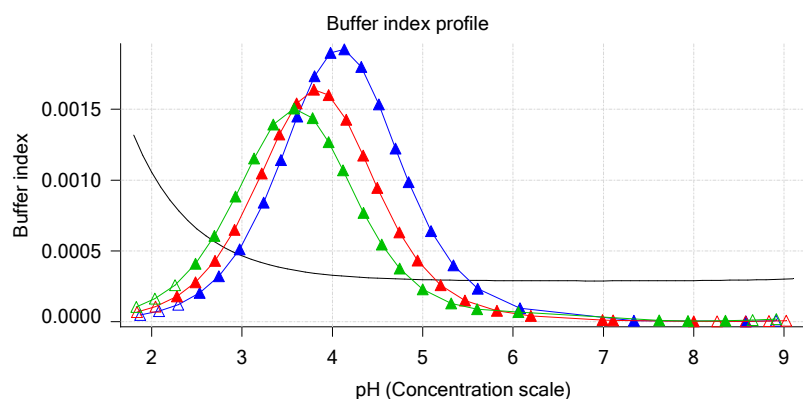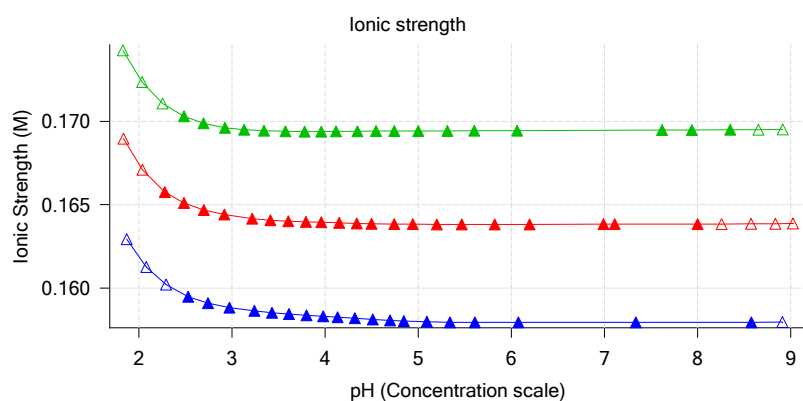
Errors   None
Warnings None

Sample logD and percent species

pH	M09_octanol logD	M09_octanol M09_octanolH	M09_octanol M09_octanol	M09_octanol M09_octanolH*	M09_octanol M09_octanol*	Comment
1.000	0.92	10.79 %	0.00 %	88.69 %	0.52 %	
1.200	0.92	10.76 %	0.00 %	88.42 %	0.82 %	Stomach pH
2.000	0.94	10.31 %	0.00 %	84.72 %	4.96 %	
3.000	1.11	7.13 %	0.03 %	58.56 %	34.29 %	
4.000	1.73	1.74 %	0.07 %	14.32 %	83.86 %	
5.000	2.54	0.20 %	0.09 %	1.67 %	98.03 %	
6.000	2.96	0.02 %	0.09 %	0.17 %	99.72 %	
6.500	3.02	0.01 %	0.09 %	0.05 %	99.85 %	
7.000	3.04	0.00 %	0.09 %	0.02 %	99.89 %	
7.400	3.05	0.00 %	0.09 %	0.01 %	99.90 %	Blood pH
8.000	3.05	0.00 %	0.09 %	0.00 %	99.91 %	
9.000	3.05	0.00 %	0.09 %	0.00 %	99.91 %	
10.000	3.05	0.00 %	0.09 %	0.00 %	99.91 %	
11.000	3.05	0.00 %	0.09 %	0.00 %	99.91 %	
12.000	3.05	0.00 %	0.09 %	0.00 %	99.91 %	

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06007**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 3:40:58 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Graphs

Charge balance residuals

Ionic strength

Buffer index profile

Sample M09_octanol Ionisation Graph

Distribution of species for sample M09_octanol

Lipophilicity Profile

Log R Profile

Sample Carbonate Ionisation Graph

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06007**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 3:40:58 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Graphs (continued)

Distribution of species for sample Carbonate

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06007**
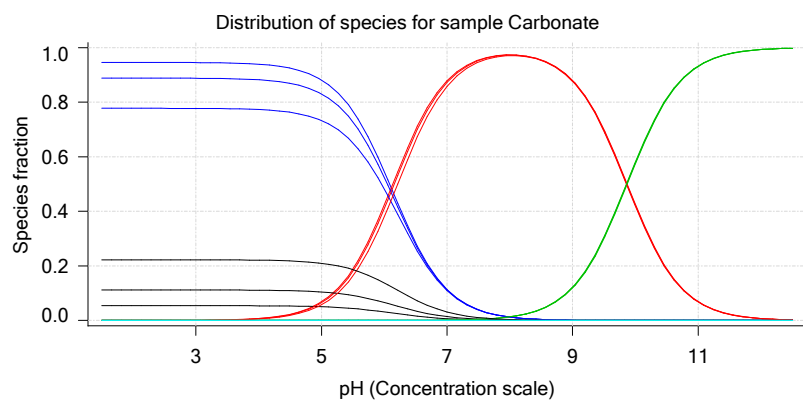Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 3:40:58 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric high logP   Titration 1 of 3   18C-06007 Points 1 to 23

Overall results

RMSD	0.369
Average ionic strength	0.158 M
Average temperature	24.9°C
Partition ratio	0.0185 : 1
Analyte concentration range	3130.9 µM to 3230.2 µM
Total points considered	19 of 23

Warnings and errors

Errors   None
Warnings   None

Four-Plus parameters

🔒	Alpha	0.124	3/6/2018 3:40:58 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r
🔒	S	0.9973	3/6/2018 3:40:58 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r
🔒	jH	0.9	3/6/2018 3:40:58 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r
🔒	jOH	-0.7	3/6/2018 3:40:58 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r

Titrants

🔒	0.50 M HCl	0.989131	3/6/2018 3:40:58 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r
🔒	0.50 M KOH	0.999845	3/6/2018 3:40:58 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

🔷	M09_octanol concentration factor	1.046
🔒	M09_octanol stoichiometry	1.000
🔒	Chloride stoichiometry	1.000
🔒	Base pKa 1	5.37
🔷	logP (XH +)	0.75
🔷	logP (neutral X)	3.05

Sample graphs

Ionisation of sample M09_octanol

Distribution of species for sample M09_octanol

Sample name: **M09_octanol**   Experiment start time: **3/6/2018 3:40:58 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-06007**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**

Sample graphs (continued)

Lipophilicity Profile
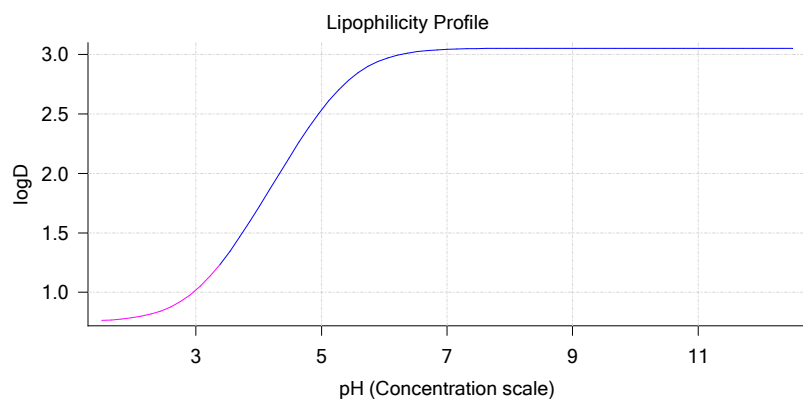
Sample logD and percent species

pH	M09_octanol logD	M09_octanol M09_octanolH	M09_octanol M09_octanol	M09_octanol M09_octanolH*	M09_octanol M09_octanol*	Comment
1.000	0.75	90.46 %	0.00 %	9.46 %	0.08 %	
1.200	0.76	90.41 %	0.01 %	9.45 %	0.13 %	Stomach pH
2.000	0.79	89.77 %	0.04 %	9.39 %	0.80 %	
3.000	1.02	83.46 %	0.36 %	8.72 %	7.46 %	
4.000	1.71	48.98 %	2.09 %	5.12 %	43.81 %	
5.000	2.53	9.55 %	4.07 %	1.00 %	85.38 %	
6.000	2.96	1.05 %	4.50 %	0.11 %	94.34 %	
6.500	3.02	0.34 %	4.54 %	0.04 %	95.09 %	
7.000	3.04	0.11 %	4.55 %	0.01 %	95.34 %	
7.400	3.05	0.04 %	4.55 %	0.00 %	95.40 %	Blood pH
8.000	3.05	0.01 %	4.55 %	0.00 %	95.44 %	
9.000	3.05	0.00 %	4.55 %	0.00 %	95.45 %	
10.000	3.05	0.00 %	4.55 %	0.00 %	95.45 %	
11.000	3.05	0.00 %	4.55 %	0.00 %	95.45 %	
12.000	3.05	0.00 %	4.55 %	0.00 %	95.45 %	

Carbonate and acidity

Carbonate   0.032 mM
Acidity error   0.097 mM

Other graphs

Assay progress

Titration graph

pH-metric

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06007**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 3:40:58 PM**
Analyst: **Pion**
Instrument ID: **T312060**
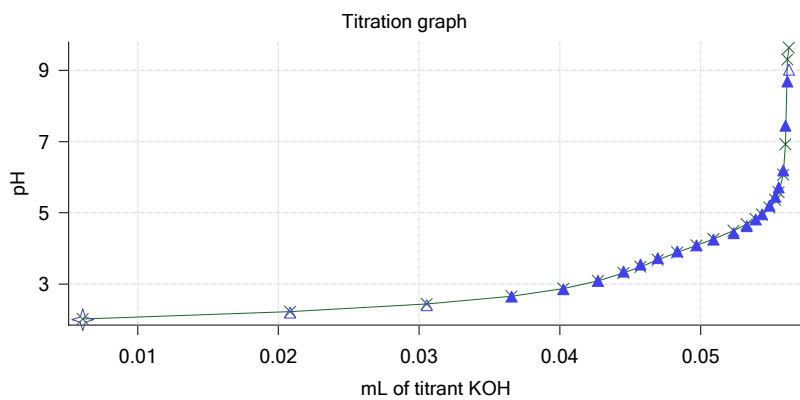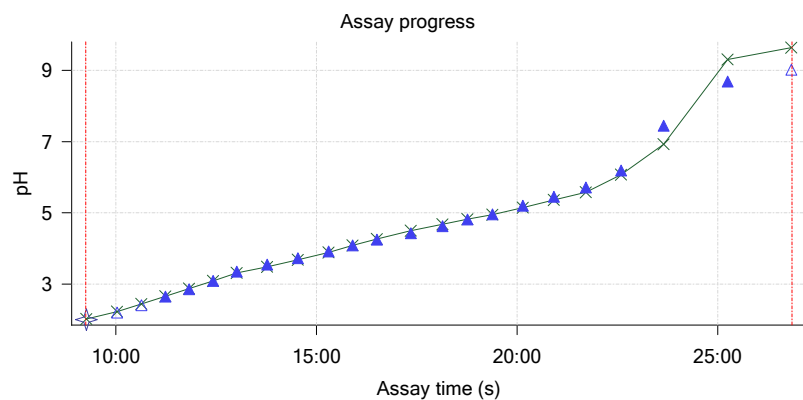
Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
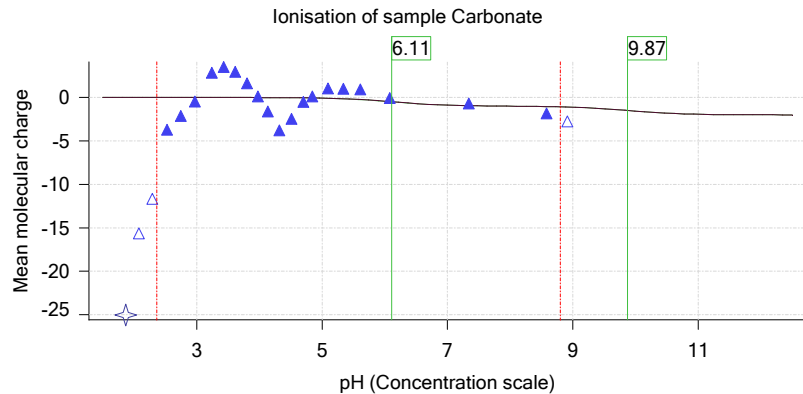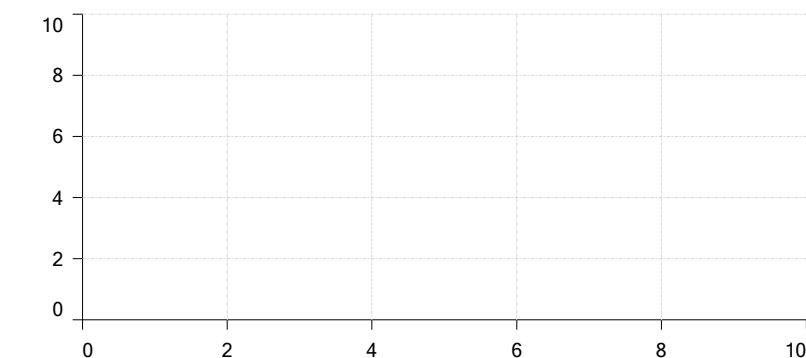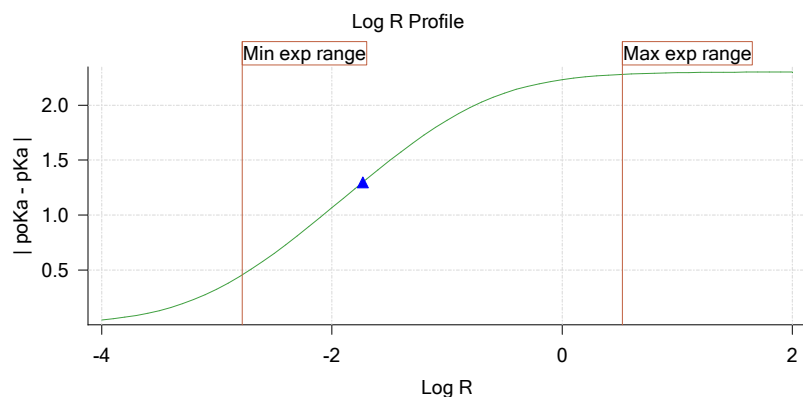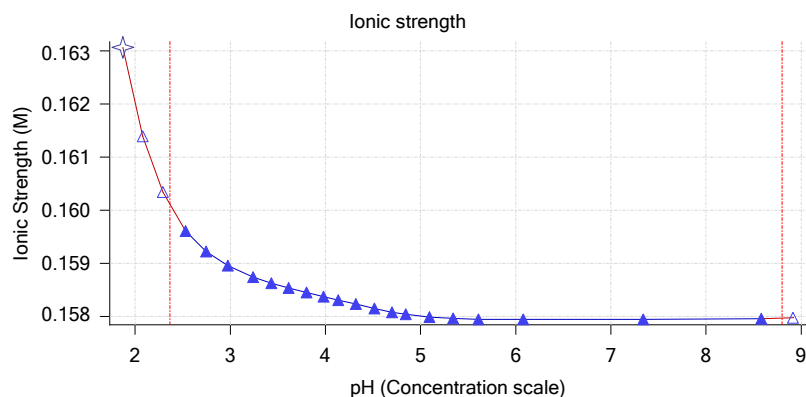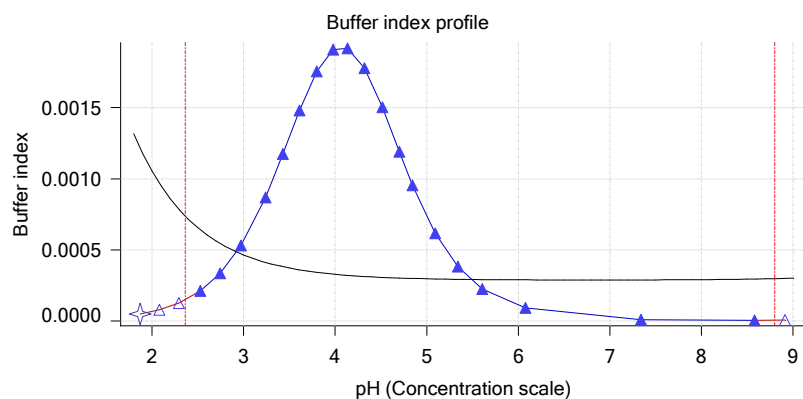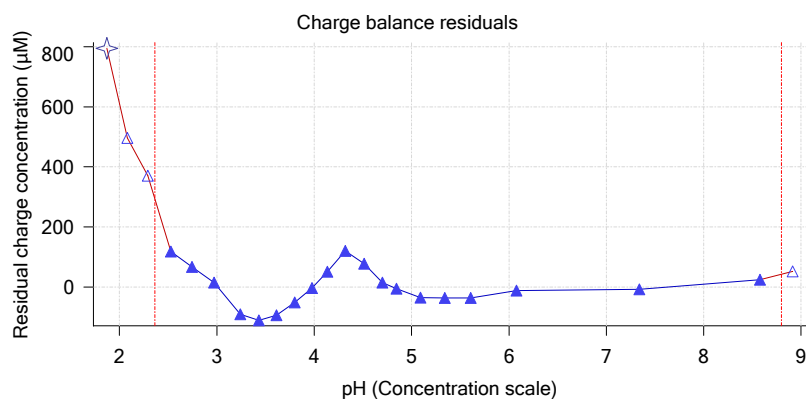
Sample name: **M09_octanol**   Experiment start time: **3/6/2018 3:40:58 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-06007**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**

pH-metric high logP   Titration 2 of 3   18C-06007 Points 24 to 50

Overall results

RMSD   0.910
Average ionic strength   0.164 M
Average temperature   25.0°C
Partition ratio   0.0407 : 1
Analyte concentration range 2862.7 µM to 2955.4 µM
Total points considered   21 of 27

Warnings and errors

Errors   None
Warnings   None

Four-Plus parameters

	Alpha	0.124	3/6/2018 3:40:58 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r
	S	0.9973	3/6/2018 3:40:58 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r
	jH	0.9	3/6/2018 3:40:58 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r
	jOH	-0.7	3/6/2018 3:40:58 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r

Titrants

	0.50 M HCl	0.989131	3/6/2018 3:40:58 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r
	0.50 M KOH	0.999845	3/6/2018 3:40:58 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M09_octanol concentration factor   0.952
M09_octanol stoichiometry   1.000
Chloride stoichiometry   1.000
Base pKa 1   5.37
logP (XH +)   0.76
logP (neutral X)   2.97

Sample graphs

Ionisation of sample M09_octanol

Distribution of species for sample M09_octanol

Sample name: **M09_octanol**　　　　　　　　Experiment start time: **3/6/2018 3:40:58 PM**
Assay name: **pH-metric high logP**　　　　　　　Analyst: **Pion**
Assay ID: **18C-06007**　　　　　　　　　　　Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**

Sample graphs (continued)

Lipophilicity Profile
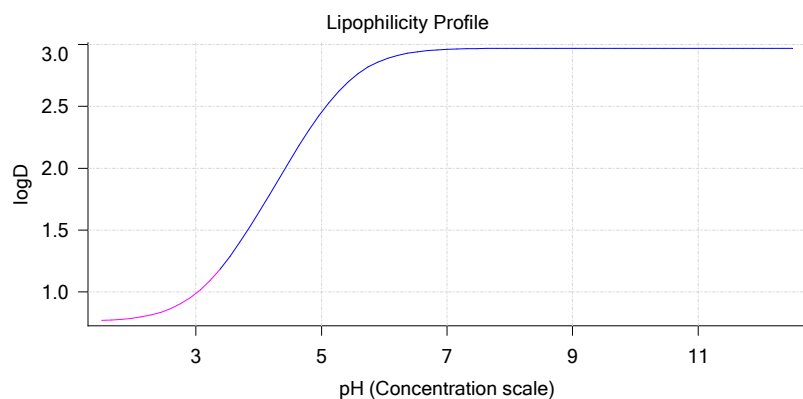
Sample logD and percent species

pH	M09_octanol logD	M09_octanol M09_octanolH	M09_octanol M09_octanol	M09_octanol M09_octanolH*	M09_octanol M09_octanol*	Comment
1.000	0.76	80.91 %	0.00 %	18.96 %	0.13 %	
1.200	0.76	80.84 %	0.01 %	18.94 %	0.21 %	Stomach pH
2.000	0.79	79.94 %	0.03 %	18.73 %	1.30 %	
3.000	0.99	71.38 %	0.30 %	16.73 %	11.59 %	
4.000	1.64	34.48 %	1.47 %	8.08 %	55.97 %	
5.000	2.45	5.59 %	2.38 %	1.31 %	90.72 %	
6.000	2.88	0.60 %	2.54 %	0.14 %	96.72 %	
6.500	2.94	0.19 %	2.55 %	0.04 %	97.21 %	
7.000	2.96	0.06 %	2.56 %	0.01 %	97.37 %	
7.400	2.97	0.02 %	2.56 %	0.01 %	97.41 %	Blood pH
8.000	2.97	0.01 %	2.56 %	0.00 %	97.43 %	
9.000	2.97	0.00 %	2.56 %	0.00 %	97.44 %	
10.000	2.97	0.00 %	2.56 %	0.00 %	97.44 %	
11.000	2.97	0.00 %	2.56 %	0.00 %	97.44 %	
12.000	2.97	0.00 %	2.56 %	0.00 %	97.44 %	

Carbonate and acidity

Carbonate　　0.026 mM
Acidity error　0.241 mM

Other graphs

Assay progress

Titration graph

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06007**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 3:40:58 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

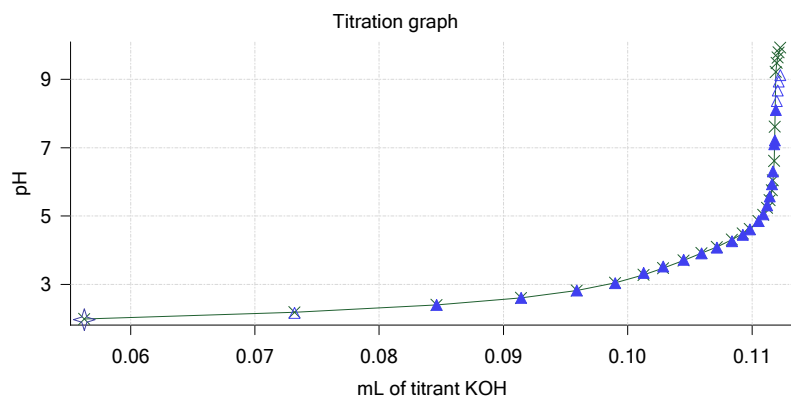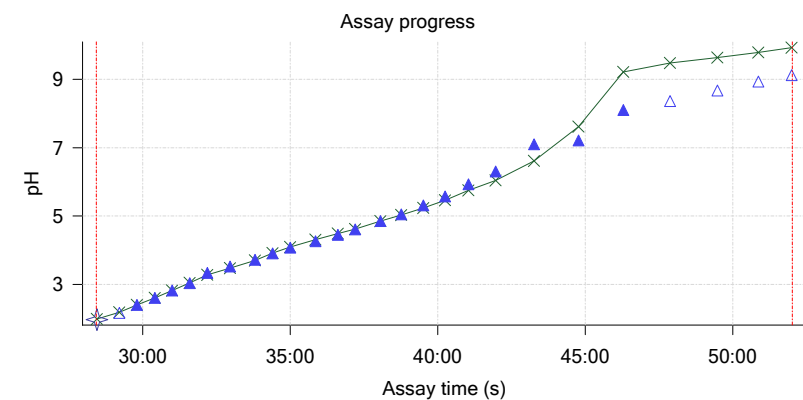### Ionic strength

Log R Profile

Ionisation of sample Carbonate
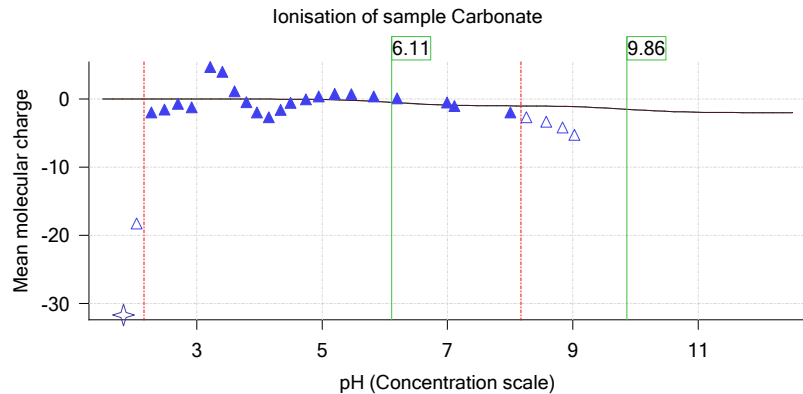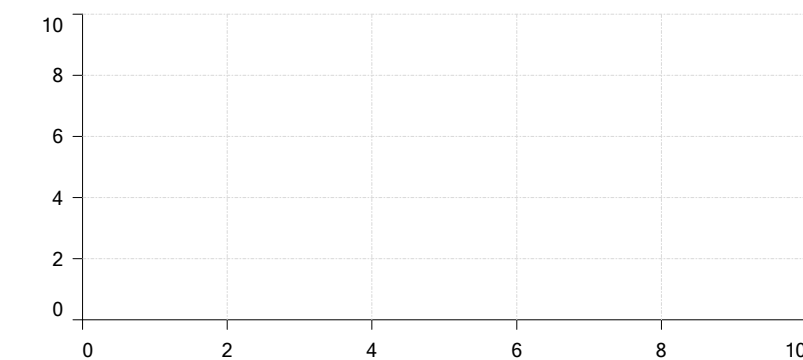
Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06007**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 3:40:58 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric high logP   Titration 3 of 3   18C-06007 Points 51 to 74

Overall results

RMSD	0.405
Average ionic strength	0.170 M
Average temperature	25.0°C
Partition ratio	0.0926 : 1
Analyte concentration range	2547.3 µM to 2626.2 µM
Total points considered	19 of 24

Warnings and errors

Errors   None
Warnings None

Four-Plus parameters

	Alpha	0.124	3/6/2018 3:40:58 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r
	S	0.9973	3/6/2018 3:40:58 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r
	jH	0.9	3/6/2018 3:40:58 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r
	jOH	-0.7	3/6/2018 3:40:58 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r

Titrants

	0.50 M HCl	0.989131	3/6/2018 3:40:58 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r
	0.50 M KOH	0.999845	3/6/2018 3:40:58 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M09_octanol concentration factor	0.937
M09_octanol stoichiometry	1.000
Chloride stoichiometry	1.000
Base pKa 1	5.37
logP (XH +)	0.76
logP (neutral X)	3.01

Sample graphs

Ionisation of sample M09_octanol

Distribution of species for sample M09_octanol

Sample graphs (continued)

Lipophilicity Profile

Sample logD and percent species

pH	M09_octanol logD	M09_octanol M09_octanolH	M09_octanol M09_octanol	M09_octanol M09_octanolH*	M09_octanol M09_octanol*	Comment
1.000	0.76	65.23 %	0.00 %	34.50 %	0.27 %	
1.200	0.76	65.13 %	0.00 %	34.45 %	0.42 %	Stomach pH
2.000	0.79	63.69 %	0.03 %	33.69 %	2.60 %	
3.000	1.00	51.51 %	0.22 %	27.25 %	21.02 %	
4.000	1.68	17.69 %	0.75 %	9.36 %	72.19 %	
5.000	2.50	2.34 %	1.00 %	1.24 %	95.43 %	
6.000	2.92	0.24 %	1.03 %	0.13 %	98.60 %	
6.500	2.98	0.08 %	1.03 %	0.04 %	98.85 %	
7.000	3.00	0.02 %	1.03 %	0.01 %	98.93 %	
7.400	3.01	0.01 %	1.03 %	0.01 %	98.95 %	Blood pH
8.000	3.01	0.00 %	1.03 %	0.00 %	98.96 %	
9.000	3.01	0.00 %	1.03 %	0.00 %	98.97 %	
10.000	3.01	0.00 %	1.03 %	0.00 %	98.97 %	
11.000	3.01	0.00 %	1.03 %	0.00 %	98.97 %	
12.000	3.01	0.00 %	1.03 %	0.00 %	98.97 %	

Carbonate and acidity

Carbonate   0.086 mM
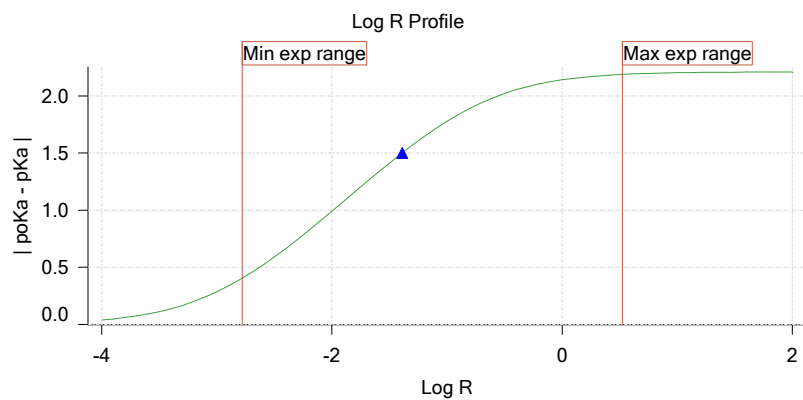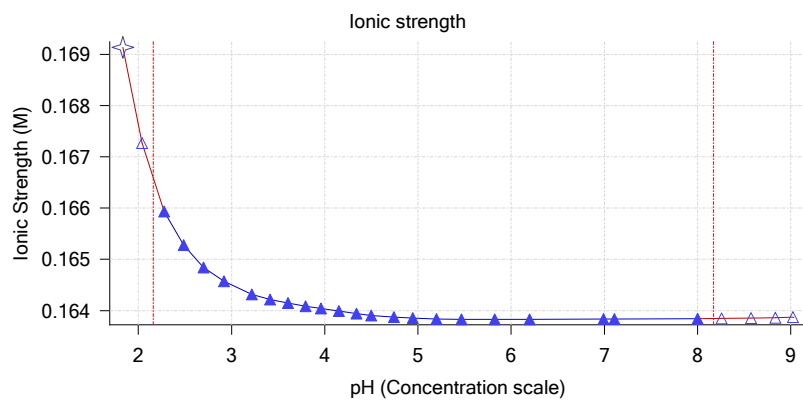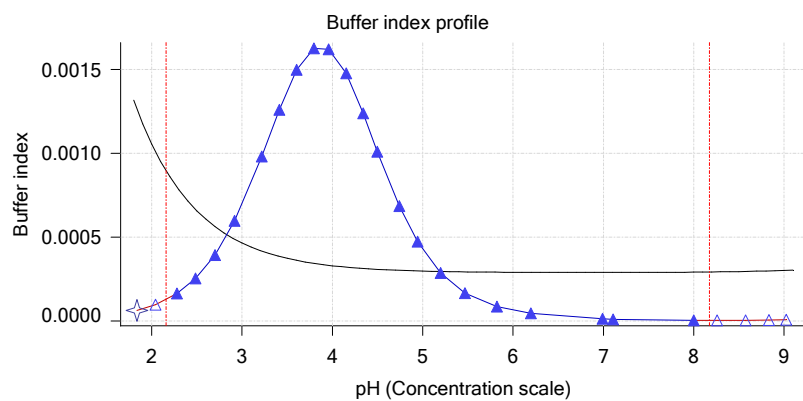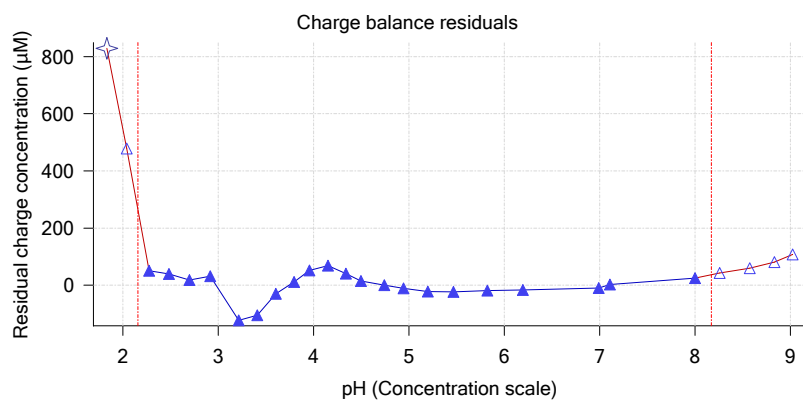Acidity error   0.305 mM

Other graphs

Assay progress

Titration graph

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06007**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 3:40:58 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
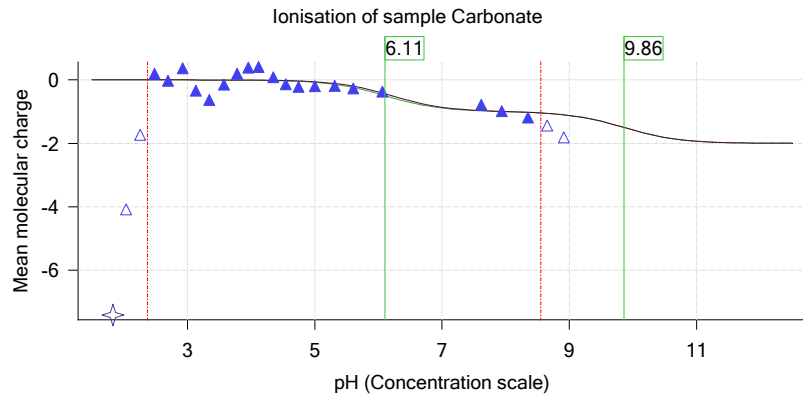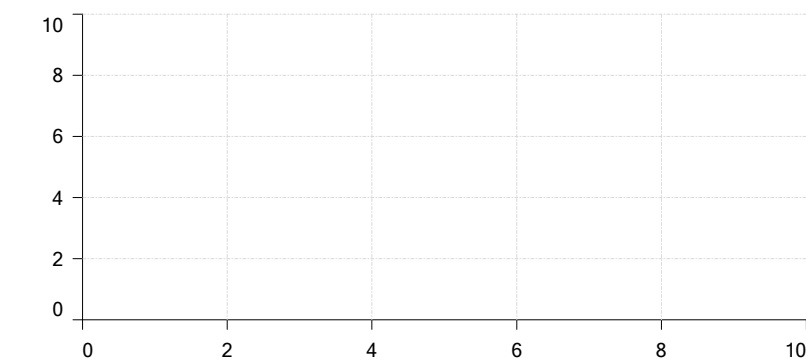
Sample name: **M09_octanol** Experiment start time: **3/6/2018 3:40:58 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-06007** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M09_octanol	2/27/2018 4:56:17 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001470 g	3/6/2018 3:39:12 PM	User entered value
Formula weight	287.74 g/mol	2/27/2018 4:45:45 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	251.28	2/27/2018 4:45:45 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	2/27/2018 4:45:45 PM	User entered value
Sample is a	Base	2/27/2018 4:45:45 PM	User entered value
pKa 1	5.37	2/27/2018 4:45:45 PM	User entered value
logp (XH +)	0.76	3/2/2018 3:27:23 PM	User entered value
logP (neutral X)	3.27	3/2/2018 3:27:17 PM	User entered value
Stoichiometry	1.00000		Default value
Aprotic counterion name	Chloride		From standards.xml file
Stoichiometry	1.00		From standards.xml file
Charge per counterion	-1		From standards.xml file

Events

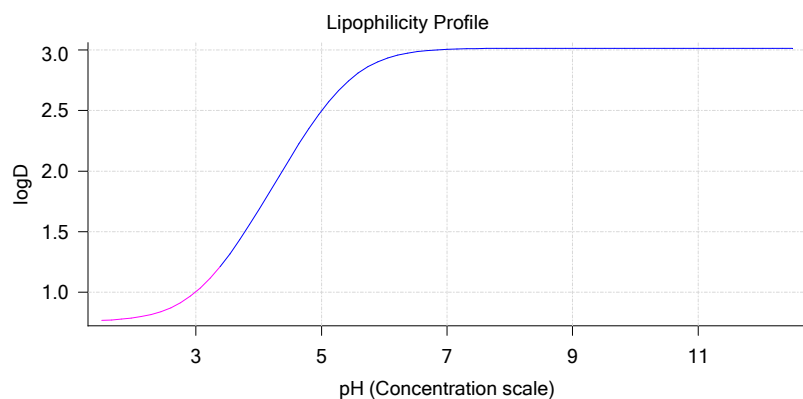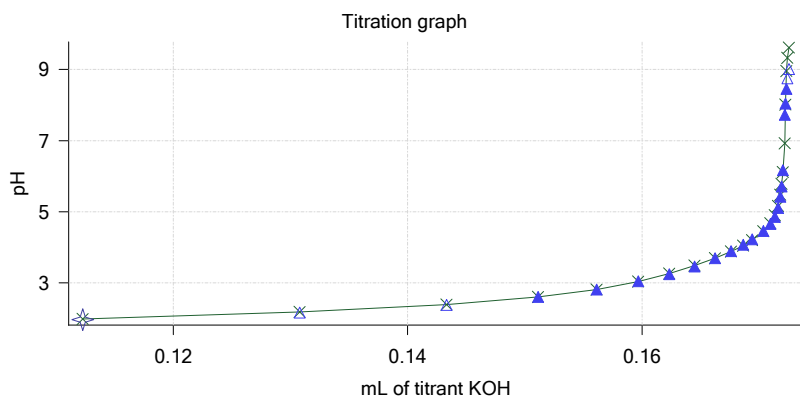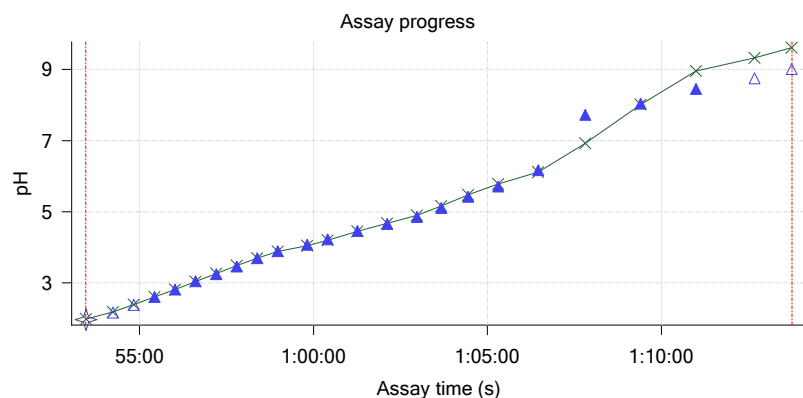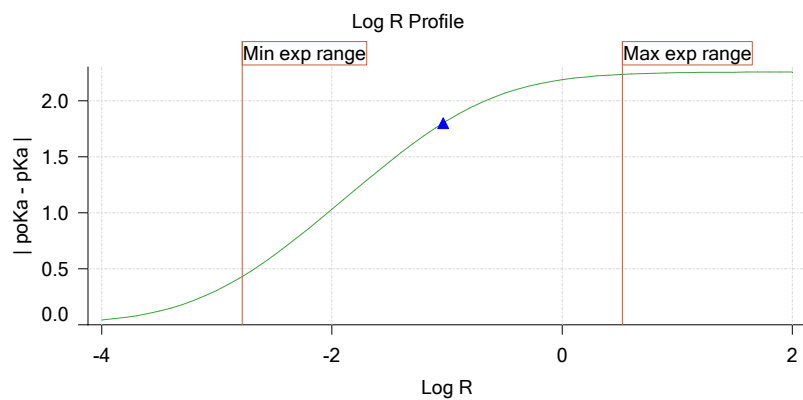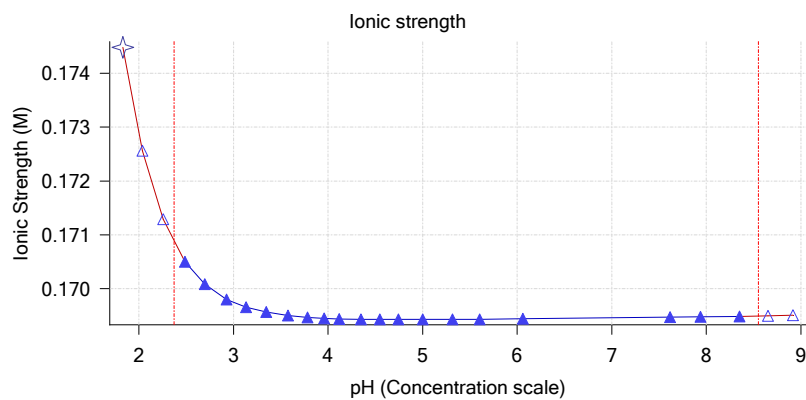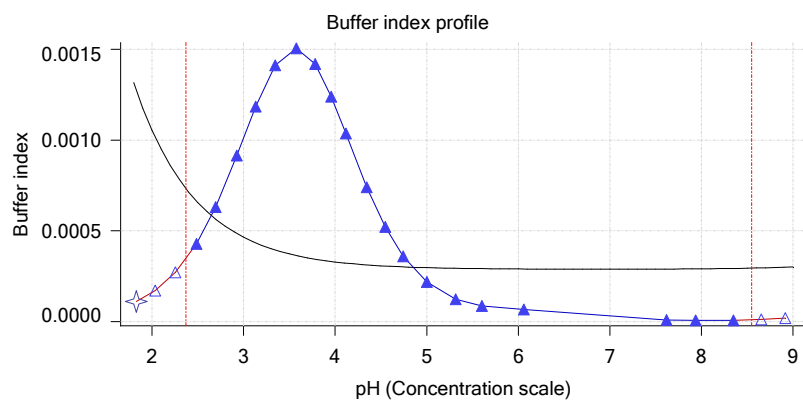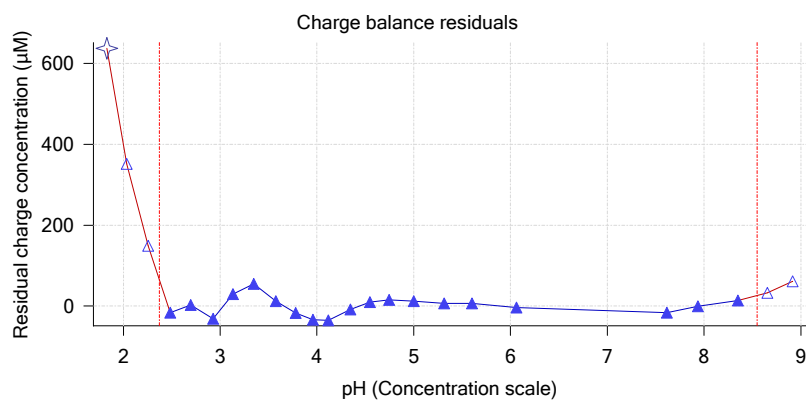| Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
6:16.5	Initial pH = 3.92									
9:16.0	Data point 1	1.50000 mL	0.04544 mL	0.00609 mL	0.03001 mL	2.003	-0.00765	0.85441	0.00041	10.0 s
10:02.2	Data point 2	1.50000 mL	0.04544 mL	0.02084 mL	0.03001 mL	2.206	-0.00581	0.82838	0.00032	10.5 s
10:38.4	Data point 3	1.50000 mL	0.04544 mL	0.03053 mL	0.03001 mL	2.415	-0.00308	0.68547	0.00018	10.5 s
11:14.3	Data point 4	1.50000 mL	0.04544 mL	0.03657 mL	0.03001 mL	2.649	-0.00951	0.26483	0.00091	10.0 s
11:49.8	Data point 5	1.50000 mL	0.04544 mL	0.04024 mL	0.03001 mL	2.863	-0.01634	0.89001	0.00086	10.0 s
12:25.3	Data point 6	1.50000 mL	0.04544 mL	0.04271 mL	0.03001 mL	3.089	-0.00759	0.82120	0.00041	10.0 s
13:00.8	Data point 7	1.50000 mL	0.04544 mL	0.04452 mL	0.03001 mL	3.357	-0.00824	0.86493	0.00044	10.0 s
13:46.4	Data point 8	1.50000 mL	0.04544 mL	0.04572 mL	0.03001 mL	3.546	-0.00997	0.85301	0.00053	10.0 s
14:32.2	Data point 9	1.50000 mL	0.04544 mL	0.04694 mL	0.03001 mL	3.727	-0.00887	0.87089	0.00047	10.5 s
15:18.4	Data point 10	1.50000 mL	0.04544 mL	0.04833 mL	0.03001 mL	3.916	-0.01261	0.86654	0.00067	10.0 s
15:54.0	Data point 11	1.50000 mL	0.04544 mL	0.04969 mL	0.03001 mL	4.093	-0.01852	0.93335	0.00095	11.0 s
16:30.4	Data point 12	1.50000 mL	0.04544 mL	0.05092 mL	0.03001 mL	4.247	-0.01783	0.96763	0.00090	10.0 s
17:21.2	Data point 13	1.50000 mL	0.04544 mL	0.05233 mL	0.03001 mL	4.433	-0.01718	0.93747	0.00088	11.5 s
18:08.5	Data point 14	1.50000 mL	0.04544 mL	0.05327 mL	0.03001 mL	4.627	-0.01904	0.93322	0.00097	12.0 s
18:45.9	Data point 15	1.50000 mL	0.04544 mL	0.05390 mL	0.03001 mL	4.812	-0.01725	0.84669	0.00093	12.0 s
19:23.3	Data point 16	1.50000 mL	0.04544 mL	0.05435 mL	0.03001 mL	4.956	-0.01847	0.93434	0.00094	15.0 s
20:08.9	Data point 17	1.50000 mL	0.04544 mL	0.05489 mL	0.03001 mL	5.203	-0.01881	0.92505	0.00097	16.0 s
20:55.1	Data point 18	1.50000 mL	0.04544 mL	0.05529 mL	0.03001 mL	5.450	-0.01772	0.88375	0.00093	17.5 s
21:43.1	Data point 19	1.50000 mL	0.04544 mL	0.05555 mL	0.03001 mL	5.717	-0.01934	0.94249	0.00098	17.0 s
22:35.7	Data point 20	1.50000 mL	0.04544 mL	0.05586 mL	0.03001 mL	6.186	-0.01984	0.97180	0.00099	33.0 s
23:39.3	Data point 21	1.50000 mL	0.04544 mL	0.05602 mL	0.03001 mL	7.443	-0.10565	0.99712	0.00522	Timed out at 59.5 s
25:15.0	Data point 22	1.50000 mL	0.04544 mL	0.05616 mL	0.03001 mL	8.681	-0.01903	0.92118	0.00098	59.5 s
26:50.1	Data point 23	1.50000 mL	0.04544 mL	0.05628 mL	0.03001 mL	9.012	-0.01984	0.96660	0.00100	37.5 s
28:26.7	Data point 24	1.50000 mL	0.10228 mL	0.05628 mL	0.07001 mL	1.967	-0.00938	0.82269	0.00051	10.0 s
29:12.7	Data point 25	1.50000 mL	0.10228 mL	0.07319 mL	0.07001 mL	2.167	-0.00239	0.33662	0.00020	10.0 s
29:48.4	Data point 26	1.50000 mL	0.10228 mL	0.08462 mL	0.07001 mL	2.401	-0.00220	0.08165	0.00038	10.5 s
30:24.5	Data point 27	1.50000 mL	0.10228 mL	0.09142 mL	0.07001 mL	2.605	-0.00054	0.07623	0.00010	10.0 s
31:00.1	Data point 28	1.50000 mL	0.10228 mL	0.09591 mL	0.07001 mL	2.819	-0.00633	0.20637	0.00069	10.0 s
31:35.6	Data point 29	1.50000 mL	0.10228 mL	0.09899 mL	0.07001 mL	3.036	-0.01322	0.81377	0.00072	10.5 s
32:11.6	Data point 30	1.50000 mL	0.10228 mL	0.10129 mL	0.07001 mL	3.333	-0.00473	0.38455	0.00038	10.0 s
32:57.3	Data point 31	1.50000 mL	0.10228 mL	0.10285 mL	0.07001 mL	3.527	-0.00844	0.34234	0.00071	10.0 s
33:48.3	Data point 32	1.50000 mL	0.10228 mL	0.10449 mL	0.07001 mL	3.721	-0.01104	0.52367	0.00075	10.5 s
34:24.3	Data point 33	1.50000 mL	0.10228 mL	0.10595 mL	0.07001 mL	3.910	-0.00623	0.66641	0.00038	10.0 s
34:59.8	Data point 34	1.50000 mL	0.10228 mL	0.10717 mL	0.07001 mL	4.073	-0.00589	0.76350	0.00033	10.5 s
35:51.2	Data point 35	1.50000 mL	0.10228 mL	0.10840 mL	0.07001 mL	4.265	-0.01218	0.79615	0.00067	10.0 s

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06007**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 3:40:58 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
36:36.9	Data point 36	1.50000 mL	0.10228 mL	0.10927 mL	0.07001 mL	4.453	-0.01574	0.77656	0.00088	10.0 s
37:12.3	Data point 37	1.50000 mL	0.10228 mL	0.10983 mL	0.07001 mL	4.611	-0.01114	0.70830	0.00065	10.5 s
38:03.7	Data point 38	1.50000 mL	0.10228 mL	0.11054 mL	0.07001 mL	4.855	-0.01503	0.83195	0.00081	11.5 s
38:45.7	Data point 39	1.50000 mL	0.10228 mL	0.11091 mL	0.07001 mL	5.055	-0.00135	0.00984	0.00067	14.5 s
39:30.9	Data point 40	1.50000 mL	0.10228 mL	0.11122 mL	0.07001 mL	5.310	-0.01935	0.93748	0.00099	13.5 s
40:15.0	Data point 41	1.50000 mL	0.10228 mL	0.11143 mL	0.07001 mL	5.577	-0.01835	0.93150	0.00094	17.0 s
41:02.4	Data point 42	1.50000 mL	0.10228 mL	0.11160 mL	0.07001 mL	5.932	-0.01854	0.95517	0.00094	25.0 s
41:58.0	Data point 43	1.50000 mL	0.10228 mL	0.11169 mL	0.07001 mL	6.304	-0.01938	0.96132	0.00098	47.5 s
43:16.1	Data point 44	1.50000 mL	0.10228 mL	0.11178 mL	0.07001 mL	7.096	-0.08353	0.99184	0.00414	Timed out at 59.5 s
44:46.6	Data point 45	1.50000 mL	0.10228 mL	0.11183 mL	0.07001 mL	7.214	-0.05929	0.99332	0.00294	Timed out at 59.5 s
46:17.1	Data point 46	1.50000 mL	0.10228 mL	0.11192 mL	0.07001 mL	8.104	-0.05533	0.99034	0.00275	Timed out at 59.5 s
47:52.7	Data point 47	1.50000 mL	0.10228 mL	0.11199 mL	0.07001 mL	8.361	-0.02231	0.99013	0.00111	Timed out at 59.5 s
49:28.4	Data point 48	1.50000 mL	0.10228 mL	0.11207 mL	0.07001 mL	8.675	-0.01974	0.96662	0.00099	43.0 s
50:52.3	Data point 49	1.50000 mL	0.10228 mL	0.11216 mL	0.07001 mL	8.935	-0.01905	0.95683	0.00096	32.0 s
51:60.0	Data point 50	1.50000 mL	0.10228 mL	0.11228 mL	0.07001 mL	9.123	-0.01924	0.93622	0.00098	27.5 s
53:28.1	Data point 51	1.50000 mL	0.16298 mL	0.11228 mL	0.17001 mL	1.963	-0.00291	0.11888	0.00042	10.0 s
54:14.4	Data point 52	1.50000 mL	0.16298 mL	0.13079 mL	0.17001 mL	2.162	-0.00496	0.56826	0.00032	10.0 s
54:50.1	Data point 53	1.50000 mL	0.16298 mL	0.14332 mL	0.17001 mL	2.380	-0.01003	0.32764	0.00087	10.0 s
55:25.7	Data point 54	1.50000 mL	0.16298 mL	0.15113 mL	0.17001 mL	2.605	-0.00142	0.12787	0.00020	10.0 s
56:01.3	Data point 55	1.50000 mL	0.16298 mL	0.15614 mL	0.17001 mL	2.814	-0.00875	0.26635	0.00084	10.0 s
56:36.8	Data point 56	1.50000 mL	0.16298 mL	0.15969 mL	0.17001 mL	3.044	-0.00319	0.61153	0.00020	10.0 s
57:12.3	Data point 57	1.50000 mL	0.16298 mL	0.16232 mL	0.17001 mL	3.248	-0.01113	0.63073	0.00069	10.0 s
57:47.8	Data point 58	1.50000 mL	0.16298 mL	0.16449 mL	0.17001 mL	3.462	-0.00502	0.86633	0.00027	10.0 s
58:23.2	Data point 59	1.50000 mL	0.16298 mL	0.16625 mL	0.17001 mL	3.691	-0.01227	0.89636	0.00064	10.0 s
58:58.6	Data point 60	1.50000 mL	0.16298 mL	0.16761 mL	0.17001 mL	3.895	-0.01553	0.75391	0.00088	25.0 s
59:49.0	Data point 61	1.50000 mL	0.16298 mL	0.16863 mL	0.17001 mL	4.072	-0.01667	0.79855	0.00092	10.0 s
1:00:24.5	Data point 62	1.50000 mL	0.16298 mL	0.16940 mL	0.17001 mL	4.230	-0.00448	0.66946	0.00027	10.5 s
1:01:15.9	Data point 63	1.50000 mL	0.16298 mL	0.17037 mL	0.17001 mL	4.459	-0.00209	0.01107	0.00098	10.5 s
1:02:07.3	Data point 64	1.50000 mL	0.16298 mL	0.17096 mL	0.17001 mL	4.659	-0.01788	0.81862	0.00098	10.5 s
1:02:58.6	Data point 65	1.50000 mL	0.16298 mL	0.17133 mL	0.17001 mL	4.856	-0.01893	0.90105	0.00099	11.0 s
1:03:40.2	Data point 66	1.50000 mL	0.16298 mL	0.17161 mL	0.17001 mL	5.111	-0.01888	0.92060	0.00097	16.0 s
1:04:26.8	Data point 67	1.50000 mL	0.16298 mL	0.17180 mL	0.17001 mL	5.425	-0.01926	0.91497	0.00099	21.0 s
1:05:18.4	Data point 68	1.50000 mL	0.16298 mL	0.17192 mL	0.17001 mL	5.713	-0.01897	0.89914	0.00099	38.5 s
1:06:27.4	Data point 69	1.50000 mL	0.16298 mL	0.17201 mL	0.17001 mL	6.169	-0.01908	0.94473	0.00097	50.5 s
1:07:48.5	Data point 70	1.50000 mL	0.16298 mL	0.17218 mL	0.17001 mL	7.721	-0.10780	0.99169	0.00535	Timed out at 59.5 s
1:09:24.1	Data point 71	1.50000 mL	0.16298 mL	0.17225 mL	0.17001 mL	8.041	-0.05145	0.99163	0.00255	Timed out at 59.5 s
1:10:59.7	Data point 72	1.50000 mL	0.16298 mL	0.17232 mL	0.17001 mL	8.452	-0.02336	0.95422	0.00118	Timed out at 59.5 s
1:12:40.5	Data point 73	1.50000 mL	0.16298 mL	0.17241 mL	0.17001 mL	8.754	-0.01965	0.97546	0.00098	28.0 s
1:13:44.2	Data point 74	1.50000 mL	0.16298 mL	0.17255 mL	0.17001 mL	9.015	-0.01623	0.82712	0.00088	23.0 s
1:14:16.2	Assay volumes	1.50000 mL	0.16298 mL	0.17255 mL	0.17001 mL					

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06007**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 3:40:58 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Pion			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	9.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.030 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	120 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.040 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M09_octanol**	Experiment start time: **3/6/2018 3:40:58 PM**
Assay name: **pH-metric high logP**	Analyst: **Pion**
Assay ID: **18C-06007**	Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**	

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.100 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.124	3/6/2018 3:40:58 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r
Four-Plus S	0.9973	3/6/2018 3:40:58 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r
Four-Plus jH	0.9	3/6/2018 3:40:58 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r
Four-Plus jOH	-0.7	3/6/2018 3:40:58 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r
Base concentration factor	1.000	3/6/2018 3:40:58 PM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.989	3/6/2018 3:40:58 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 5:24:52 AM
Dispenser 0	Water		3/31/2009 5:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 10:05:59 AM
Dispenser 2	Acid		3/31/2009 5:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 10:27:22 AM
Dispenser 1	Base		3/31/2009 5:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 10:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 5:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 5:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	02-08-2018	3/6/2018 9:28:59 AM
Port B	Cyclohexane	11-01-17	2/27/2018 10:37:57 AM
Dispenser 3	Buffer		8/3/2010 5:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 10:18:04 AM
Dispenser 6	Octanol		10/22/2010 10:52:43 AM

Sample name: **M09_octanol**

Assay name: **pH-metric high logP**

Assay ID: **18C-06007**

Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 3:40:58 PM**

Analyst: **Pion**

Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	01-31-2018	2/27/2018 9:59:35 AM
Titrator		T3TM1200161	3/31/2009 5:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 2:01:00 PM
E0 calibration	+6.73 mV		3/6/2018 3:41:43 PM
Filling solution	3M KCl	KCL097	3/6/2018 9:23:20 AM
Liquids			
Wash 1	50% IPA:50% Water		3/6/2018 9:24:32 AM
Wash 2	0.5% Trition X-100 in H20		3/6/2018 9:24:35 AM
Buffer position 1	pH7 Wash		3/6/2018 9:24:38 AM
Buffer position 2	pH 7		3/6/2018 9:24:40 AM
Storage position			3/6/2018 9:24:07 AM
Wash water	6.1e+003 mL	02-27-2018	2/27/2018 9:54:39 AM
Waste	9.4e+003 mL		11/28/2017 10:36:29 AM
Temperature controller			8/5/2010 6:35:13 AM
Turbidity detector			3/31/2009 5:24:45 AM
Spectrometer		074811	11/23/2010 11:22:28 AM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	123:01:40		11/23/2010 11:22:28 AM
Calibrated on	2/27/2018 10:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 9:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06007**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 3:40:58 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00

Experiment Log

[1:59] Air gap released for Acid (0.5 M HCl)
[2:54] Air gap created for Water (0.15 M KCl)
[2:54] Air gap created for Acid (0.5 M HCl)
[2:55] Air gap created for Base (0.5 M KOH)
[2:55] Air gap released for Water (0.15 M KCl)
[2:59] Titrator arm moved over Titration position
[2:59] Titration 1 of 3
[2:59] Adding initial titrants
[2:59] Automatically add 1.50000 mL of water
[3:24] Dispensed 1.500000 mL of Water (0.15 M KCl)
[3:28] Titrator arm moved over Drain
[6:10] Titrator arm moved to Titration position
[6:10] Argon flow rate set to 100
[6:10] Stirrer speed set to 10
[6:15] Automatically add 0.03000 mL of Octanol
[6:16] Dispensed 0.030009 mL of Octanol
[6:17] Initial pH = 3.92
[6:17] Iterative adjust 3.92 -> 2.00
[6:17] pH 3.92 -> 2.00
[6:18] Air gap released for Acid (0.5 M HCl)
[6:19] Dispensed 0.045437 mL of Acid (0.5 M HCl)
[6:24] Holding pH 2.00
[8:24] Stirrer speed set to 0
[8:24] Stirrer speed set to 50
[8:24] Iterative adjust 1.94 -> 2.00
[8:24] pH 1.94 -> 2.00
[8:25] Air gap released for Base (0.5 M KOH)
[8:26] Dispensed 0.006091 mL of Base (0.5 M KOH)
[9:16] Stirrer speed set to 0
[9:26] Datapoint id 1 collected
[9:26] Stirrer speed set to 50
[9:31] pH 2.01 -> 2.21
[9:31] Using cautious pH adjust
[9:32] Dispensed 0.007714 mL of Base (0.5 M KOH)
[9:37] Stepping pH = 2.10
[9:37] Dispensed 0.006185 mL of Base (0.5 M KOH)
[9:42] Stepping pH = 2.19
[9:42] Dispensed 0.000847 mL of Base (0.5 M KOH)
[9:47] Stepping pH = 2.21
[10:03] Stirrer speed set to 0
[10:13] Datapoint id 2 collected
[10:13] Charge balance equation is out by 4.3%

Sample name: **M09_octanol**   Experiment start time: **3/6/2018 3:40:58 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-06007**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[10:13] Stirrer speed set to 50
[10:18] pH 2.21 -> 2.41
[10:18] Using charge balance adjust
[10:19] Dispensed 0.009690 mL of Base (0.5 M KOH)
[10:39] Stirrer speed set to 0
[10:49] Datapoint id 3 collected
[10:49] Charge balance equation is out by 1.3%
[10:49] Stirrer speed set to 50
[10:54] pH 2.42 -> 2.62
[10:54] Using charge balance adjust
[10:54] Dispensed 0.006044 mL of Base (0.5 M KOH)
[11:15] Stirrer speed set to 0
[11:25] Datapoint id 4 collected
[11:25] Charge balance equation is out by 13.5%
[11:25] Stirrer speed set to 50
[11:30] pH 2.66 -> 2.86
[11:30] Using charge balance adjust
[11:30] Dispensed 0.003669 mL of Base (0.5 M KOH)
[11:50] Stirrer speed set to 0
[12:00] Datapoint id 5 collected
[12:00] Charge balance equation is out by 3.7%
[12:00] Stirrer speed set to 50
[12:05] pH 2.87 -> 3.07
[12:05] Using charge balance adjust
[12:05] Dispensed 0.002469 mL of Base (0.5 M KOH)
[12:26] Stirrer speed set to 0
[12:36] Datapoint id 6 collected
[12:36] Charge balance equation is out by 10.9%
[12:36] Stirrer speed set to 50
[12:41] pH 3.10 -> 3.30
[12:41] Using charge balance adjust
[12:41] Dispensed 0.001811 mL of Base (0.5 M KOH)
[13:01] Stirrer speed set to 0
[13:11] Datapoint id 7 collected
[13:11] Charge balance equation is out by 30.3%
[13:11] Stirrer speed set to 50
[13:16] pH 3.36 -> 3.56
[13:16] Using cautious pH adjust
[13:16] Dispensed 0.000753 mL of Base (0.5 M KOH)
[13:21] Stepping pH = 3.49
[13:21] Dispensed 0.000329 mL of Base (0.5 M KOH)
[13:27] Stepping pH = 3.54
[13:27] Dispensed 0.000118 mL of Base (0.5 M KOH)
[13:32] Stepping pH = 3.55
[13:47] Stirrer speed set to 0
[13:57] Datapoint id 8 collected
[13:57] Charge balance equation is out by 19.6%
[13:57] Stirrer speed set to 50
[14:02] pH 3.55 -> 3.75
[14:02] Using cautious pH adjust
[14:02] Dispensed 0.000729 mL of Base (0.5 M KOH)
[14:07] Stepping pH = 3.68
[14:07] Dispensed 0.000329 mL of Base (0.5 M KOH)
[14:12] Stepping pH = 3.72
[14:12] Dispensed 0.000165 mL of Base (0.5 M KOH)
[14:17] Stepping pH = 3.74
[14:33] Stirrer speed set to 0
[14:43] Datapoint id 9 collected
[14:43] Charge balance equation is out by 16.9%

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06007**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 3:40:58 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[14:43] Stirrer speed set to 50
[14:48] pH 3.73 -> 3.93
[14:48] Using cautious pH adjust
[14:48] Dispensed 0.000706 mL of Base (0.5 M KOH)
[14:53] Stepping pH = 3.84
[14:53] Dispensed 0.000423 mL of Base (0.5 M KOH)
[14:58] Stepping pH = 3.89
[14:59] Dispensed 0.000259 mL of Base (0.5 M KOH)
[15:04] Stepping pH = 3.92
[15:19] Stirrer speed set to 0
[15:29] Datapoint id 10 collected
[15:29] Charge balance equation is out by 2.0%
[15:29] Stirrer speed set to 50
[15:34] pH 3.92 -> 4.12
[15:34] Using charge balance adjust
[15:34] Dispensed 0.001364 mL of Base (0.5 M KOH)
[15:54] Stirrer speed set to 0
[16:05] Datapoint id 11 collected
[16:05] Charge balance equation is out by -13.7%
[16:05] Stirrer speed set to 50
[16:10] pH 4.10 -> 4.30
[16:10] Using charge balance adjust
[16:11] Dispensed 0.001223 mL of Base (0.5 M KOH)
[16:31] Stirrer speed set to 0
[16:41] Datapoint id 12 collected
[16:41] Charge balance equation is out by -26.8%
[16:41] Stirrer speed set to 50
[16:46] pH 4.25 -> 4.45
[16:46] Using cautious pH adjust
[16:46] Dispensed 0.000541 mL of Base (0.5 M KOH)
[16:51] Stepping pH = 4.33
[16:51] Dispensed 0.000541 mL of Base (0.5 M KOH)
[16:56] Stepping pH = 4.42
[16:56] Dispensed 0.000188 mL of Base (0.5 M KOH)
[17:01] Stepping pH = 4.43
[17:01] Dispensed 0.000141 mL of Base (0.5 M KOH)
[17:06] Stepping pH = 4.45
[17:22] Stirrer speed set to 0
[17:33] Datapoint id 13 collected
[17:33] Charge balance equation is out by -31.1%
[17:33] Stirrer speed set to 50
[17:38] pH 4.44 -> 4.64
[17:38] Using cautious pH adjust
[17:38] Dispensed 0.000423 mL of Base (0.5 M KOH)
[17:43] Stepping pH = 4.55
[17:43] Dispensed 0.000259 mL of Base (0.5 M KOH)
[17:49] Stepping pH = 4.59
[17:49] Dispensed 0.000259 mL of Base (0.5 M KOH)
[17:54] Stepping pH = 4.64
[18:09] Stirrer speed set to 0
[18:21] Datapoint id 14 collected
[18:21] Charge balance equation is out by -9.3%
[18:21] Stirrer speed set to 50
[18:26] pH 4.64 -> 4.84
[18:26] Using charge balance adjust
[18:26] Dispensed 0.000635 mL of Base (0.5 M KOH)
[18:46] Stirrer speed set to 0
[18:58] Datapoint id 15 collected
[18:58] Charge balance equation is out by -14.0%

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06007**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 3:40:58 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[18:58] Stirrer speed set to 50
[19:03] pH 4.83 -> 5.03
[19:03] Using charge balance adjust
[19:03] Dispensed 0.000447 mL of Base (0.5 M KOH)
[19:24] Stirrer speed set to 0
[19:39] Datapoint id 16 collected
[19:39] Charge balance equation is out by -38.2%
[19:39] Stirrer speed set to 50
[19:44] pH 4.98 -> 5.18
[19:44] Using cautious pH adjust
[19:44] Dispensed 0.000165 mL of Base (0.5 M KOH)
[19:49] Stepping pH = 5.01
[19:49] Dispensed 0.000376 mL of Base (0.5 M KOH)
[19:54] Stepping pH = 5.25
[20:09] Stirrer speed set to 0
[20:25] Datapoint id 17 collected
[20:25] Charge balance equation is out by -62.0%
[20:25] Stirrer speed set to 50
[20:30] pH 5.23 -> 5.43
[20:30] Using cautious pH adjust
[20:30] Dispensed 0.000118 mL of Base (0.5 M KOH)
[20:35] Stepping pH = 5.25
[20:35] Dispensed 0.000282 mL of Base (0.5 M KOH)
[20:40] Stepping pH = 5.49
[20:55] Stirrer speed set to 0
[21:13] Datapoint id 18 collected
[21:13] Charge balance equation is out by -85.2%
[21:13] Stirrer speed set to 50
[21:18] pH 5.49 -> 5.69
[21:18] Using cautious pH adjust
[21:18] Dispensed 0.000071 mL of Base (0.5 M KOH)
[21:23] Stepping pH = 5.50
[21:23] Dispensed 0.000188 mL of Base (0.5 M KOH)
[21:28] Stepping pH = 5.74
[21:43] Stirrer speed set to 0
[22:00] Datapoint id 19 collected
[22:00] Charge balance equation is out by -94.3%
[22:00] Stirrer speed set to 50
[22:06] pH 5.76 -> 5.96
[22:06] Using cautious pH adjust
[22:06] Dispensed 0.000047 mL of Base (0.5 M KOH)
[22:11] Stepping pH = 5.77
[22:11] Dispensed 0.000141 mL of Base (0.5 M KOH)
[22:16] Stepping pH = 5.85
[22:16] Dispensed 0.000118 mL of Base (0.5 M KOH)
[22:21] Stepping pH = 6.19
[22:36] Stirrer speed set to 0
[23:09] Datapoint id 20 collected
[23:09] Charge balance equation is out by -210.5%
[23:09] Stirrer speed set to 50
[23:14] pH 6.23 -> 6.43
[23:14] Using cautious pH adjust
[23:14] Dispensed 0.000024 mL of Base (0.5 M KOH)
[23:19] Stepping pH = 6.23
[23:19] Dispensed 0.000141 mL of Base (0.5 M KOH)
[23:25] Stepping pH = 7.24
[23:40] Stirrer speed set to 0
[24:40] Datapoint id 21 collected
[24:40] Charge balance equation is out by -211.2%

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06007**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 3:40:58 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[24:40] Stirrer speed set to 50
[24:45] pH 7.39 -> 7.59
[24:45] Using cautious pH adjust
[24:45] Dispensed 0.000024 mL of Base (0.5 M KOH)
[24:50] Stepping pH = 7.36
[24:50] Dispensed 0.000024 mL of Base (0.5 M KOH)
[24:55] Stepping pH = 7.36
[24:55] Dispensed 0.000094 mL of Base (0.5 M KOH)
[25:00] Stepping pH = 8.58
[25:15] Stirrer speed set to 0
[26:15] Datapoint id 22 collected
[26:15] Charge balance equation is out by -1,276.8%
[26:15] Stirrer speed set to 50
[26:20] pH 8.72 -> 8.92
[26:20] Using cautious pH adjust
[26:20] Dispensed 0.000024 mL of Base (0.5 M KOH)
[26:25] Stepping pH = 8.71
[26:25] Dispensed 0.000071 mL of Base (0.5 M KOH)
[26:30] Stepping pH = 8.89
[26:30] Dispensed 0.000024 mL of Base (0.5 M KOH)
[26:35] Stepping pH = 9.02
[26:50] Stirrer speed set to 0
[27:28] Datapoint id 23 collected
[27:28] Charge balance equation is out by -331.4%
[27:28] Titration 2 of 3
[27:28] Adding initial titrants
[27:28] Automatically add 0.04000 mL of Octanol
[27:29] Dispensed 0.040005 mL of Octanol
[27:29] Stirrer speed set to 10
[27:30] Stirrer speed set to 55
[27:30] Iterative adjust 9.02 -> 2.00
[27:30] pH 9.02 -> 2.00
[27:31] Dispensed 0.054351 mL of Acid (0.5 M HCl)
[27:36] pH 2.02 -> 2.00
[27:37] Dispensed 0.002493 mL of Acid (0.5 M HCl)
[28:27] Stirrer speed set to 0
[28:37] Datapoint id 24 collected
[28:37] Stirrer speed set to 55
[28:42] pH 1.97 -> 2.17
[28:42] Using cautious pH adjust
[28:42] Dispensed 0.009149 mL of Base (0.5 M KOH)
[28:47] Stepping pH = 2.07
[28:48] Dispensed 0.005691 mL of Base (0.5 M KOH)
[28:53] Stepping pH = 2.14
[28:53] Dispensed 0.002070 mL of Base (0.5 M KOH)
[28:58] Stepping pH = 2.17
[29:13] Stirrer speed set to 0
[29:23] Datapoint id 25 collected
[29:23] Charge balance equation is out by 7.6%
[29:23] Stirrer speed set to 55
[29:28] pH 2.17 -> 2.37
[29:28] Using charge balance adjust
[29:29] Dispensed 0.011430 mL of Base (0.5 M KOH)
[29:49] Stirrer speed set to 0
[29:59] Datapoint id 26 collected
[29:59] Charge balance equation is out by 13.7%
[29:59] Stirrer speed set to 55
[30:04] pH 2.41 -> 2.61
[30:04] Using charge balance adjust

Sample name: **M09_octanol** Experiment start time: **3/6/2018 3:40:58 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-06007** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[30:05] Dispensed 0.006797 mL of Base (0.5 M KOH)
[30:25] Stirrer speed set to 0
[30:35] Datapoint id 27 collected
[30:35] Charge balance equation is out by -1.0%
[30:35] Stirrer speed set to 55
[30:40] pH 2.61 -> 2.81
[30:40] Using charge balance adjust
[30:40] Dispensed 0.004492 mL of Base (0.5 M KOH)
[31:00] Stirrer speed set to 0
[31:10] Datapoint id 28 collected
[31:10] Charge balance equation is out by 4.7%
[31:10] Stirrer speed set to 55
[31:16] pH 2.82 -> 3.02
[31:16] Using charge balance adjust
[31:16] Dispensed 0.003081 mL of Base (0.5 M KOH)
[31:36] Stirrer speed set to 0
[31:46] Datapoint id 29 collected
[31:46] Charge balance equation is out by 6.2%
[31:46] Stirrer speed set to 55
[31:52] pH 3.04 -> 3.24
[31:52] Using charge balance adjust
[31:52] Dispensed 0.002305 mL of Base (0.5 M KOH)
[32:12] Stirrer speed set to 0
[32:22] Datapoint id 30 collected
[32:22] Charge balance equation is out by 46.1%
[32:22] Stirrer speed set to 55
[32:27] pH 3.34 -> 3.54
[32:27] Using cautious pH adjust
[32:27] Dispensed 0.000917 mL of Base (0.5 M KOH)
[32:32] Stepping pH = 3.46
[32:32] Dispensed 0.000447 mL of Base (0.5 M KOH)
[32:37] Stepping pH = 3.51
[32:37] Dispensed 0.000188 mL of Base (0.5 M KOH)
[32:43] Stepping pH = 3.53
[32:58] Stirrer speed set to 0
[33:08] Datapoint id 31 collected
[33:08] Charge balance equation is out by 15.3%
[33:08] Stirrer speed set to 55
[33:13] pH 3.53 -> 3.73
[33:13] Using cautious pH adjust
[33:13] Dispensed 0.000823 mL of Base (0.5 M KOH)
[33:18] Stepping pH = 3.64
[33:18] Dispensed 0.000494 mL of Base (0.5 M KOH)
[33:23] Stepping pH = 3.70
[33:23] Dispensed 0.000212 mL of Base (0.5 M KOH)
[33:28] Stepping pH = 3.72
[33:28] Dispensed 0.000118 mL of Base (0.5 M KOH)
[33:34] Stepping pH = 3.73
[33:49] Stirrer speed set to 0
[33:59] Datapoint id 32 collected
[33:59] Charge balance equation is out by -0.4%
[33:59] Stirrer speed set to 55
[34:04] pH 3.72 -> 3.92
[34:04] Using charge balance adjust
[34:04] Dispensed 0.001458 mL of Base (0.5 M KOH)
[34:25] Stirrer speed set to 0
[34:35] Datapoint id 33 collected
[34:35] Charge balance equation is out by -7.5%
[34:35] Stirrer speed set to 55

Sample name: **M09_octanol**　　　　　　　　　　　　Experiment start time: **3/6/2018 3:40:58 PM**
Assay name: **pH-metric high logP**　　　　　　　　　Analyst: **Pion**
Assay ID: **18C-06007**　　　　　　　　　　　　　　　Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[34:40] pH 3.91 -> 4.11
[34:40] Using charge balance adjust
[34:40] Dispensed 0.001223 mL of Base (0.5 M KOH)
[35:00] Stirrer speed set to 0
[35:11] Datapoint id 34 collected
[35:11] Charge balance equation is out by -20.6%
[35:11] Stirrer speed set to 55
[35:16] pH 4.08 -> 4.28
[35:16] Using cautious pH adjust
[35:16] Dispensed 0.000517 mL of Base (0.5 M KOH)
[35:21] Stepping pH = 4.16
[35:21] Dispensed 0.000470 mL of Base (0.5 M KOH)
[35:26] Stepping pH = 4.24
[35:26] Dispensed 0.000165 mL of Base (0.5 M KOH)
[35:31] Stepping pH = 4.27
[35:31] Dispensed 0.000071 mL of Base (0.5 M KOH)
[35:36] Stepping pH = 4.27
[35:51] Stirrer speed set to 0
[36:02] Datapoint id 35 collected
[36:02] Charge balance equation is out by -18.3%
[36:02] Stirrer speed set to 55
[36:07] pH 4.27 -> 4.47
[36:07] Using cautious pH adjust
[36:07] Dispensed 0.000376 mL of Base (0.5 M KOH)
[36:12] Stepping pH = 4.35
[36:12] Dispensed 0.000329 mL of Base (0.5 M KOH)
[36:17] Stepping pH = 4.42
[36:17] Dispensed 0.000165 mL of Base (0.5 M KOH)
[36:22] Stepping pH = 4.46
[36:37] Stirrer speed set to 0
[36:47] Datapoint id 36 collected
[36:47] Charge balance equation is out by -13.4%
[36:47] Stirrer speed set to 55
[36:52] pH 4.46 -> 4.66
[36:52] Using charge balance adjust
[36:52] Dispensed 0.000564 mL of Base (0.5 M KOH)
[37:13] Stirrer speed set to 0
[37:23] Datapoint id 37 collected
[37:23] Charge balance equation is out by -25.1%
[37:23] Stirrer speed set to 55
[37:28] pH 4.62 -> 4.82
[37:28] Using cautious pH adjust
[37:28] Dispensed 0.000212 mL of Base (0.5 M KOH)
[37:33] Stepping pH = 4.67
[37:34] Dispensed 0.000306 mL of Base (0.5 M KOH)
[37:39] Stepping pH = 4.79
[37:39] Dispensed 0.000047 mL of Base (0.5 M KOH)
[37:44] Stepping pH = 4.80
[37:44] Dispensed 0.000141 mL of Base (0.5 M KOH)
[37:49] Stepping pH = 4.86
[38:04] Stirrer speed set to 0
[38:16] Datapoint id 38 collected
[38:16] Charge balance equation is out by -66.8%
[38:16] Stirrer speed set to 55
[38:21] pH 4.87 -> 5.07
[38:21] Using cautious pH adjust
[38:21] Dispensed 0.000118 mL of Base (0.5 M KOH)
[38:26] Stepping pH = 4.90
[38:26] Dispensed 0.000259 mL of Base (0.5 M KOH)

Sample name: **M09_octanol**   Experiment start time: **3/6/2018 3:40:58 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-06007**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[38:31] Stepping pH = 5.07
[38:46] Stirrer speed set to 0
[39:01] Datapoint id 39 collected
[39:01] Charge balance equation is out by -50.1%
[39:01] Stirrer speed set to 55
[39:06] pH 5.08 -> 5.28
[39:06] Using cautious pH adjust
[39:06] Dispensed 0.000094 mL of Base (0.5 M KOH)
[39:11] Stepping pH = 5.10
[39:11] Dispensed 0.000212 mL of Base (0.5 M KOH)
[39:16] Stepping pH = 5.32
[39:31] Stirrer speed set to 0
[39:45] Datapoint id 40 collected
[39:45] Charge balance equation is out by -73.8%
[39:45] Stirrer speed set to 55
[39:50] pH 5.34 -> 5.54
[39:50] Using cautious pH adjust
[39:50] Dispensed 0.000047 mL of Base (0.5 M KOH)
[39:55] Stepping pH = 5.34
[39:55] Dispensed 0.000165 mL of Base (0.5 M KOH)
[40:00] Stepping pH = 5.59
[40:15] Stirrer speed set to 0
[40:32] Datapoint id 41 collected
[40:32] Charge balance equation is out by -98.5%
[40:32] Stirrer speed set to 55
[40:37] pH 5.61 -> 5.81
[40:37] Using cautious pH adjust
[40:37] Dispensed 0.000047 mL of Base (0.5 M KOH)
[40:43] Stepping pH = 5.62
[40:43] Dispensed 0.000118 mL of Base (0.5 M KOH)
[40:48] Stepping pH = 5.97
[41:03] Stirrer speed set to 0
[41:28] Datapoint id 42 collected
[41:28] Charge balance equation is out by -92.4%
[41:28] Stirrer speed set to 55
[41:33] pH 5.99 -> 6.19
[41:33] Using cautious pH adjust
[41:33] Dispensed 0.000024 mL of Base (0.5 M KOH)
[41:38] Stepping pH = 6.00
[41:38] Dispensed 0.000071 mL of Base (0.5 M KOH)
[41:43] Stepping pH = 6.30
[41:58] Stirrer speed set to 0
[42:46] Datapoint id 43 collected
[42:46] Charge balance equation is out by -90.5%
[42:46] Stirrer speed set to 55
[42:51] pH 6.33 -> 6.53
[42:51] Using cautious pH adjust
[42:51] Dispensed 0.000024 mL of Base (0.5 M KOH)
[42:56] Stepping pH = 6.35
[42:56] Dispensed 0.000071 mL of Base (0.5 M KOH)
[43:01] Stepping pH = 6.95
[43:16] Stirrer speed set to 0
[44:16] Datapoint id 44 collected
[44:16] Charge balance equation is out by -77.9%
[44:16] Stirrer speed set to 55
[44:22] pH 7.16 -> 7.36
[44:22] Using cautious pH adjust
[44:22] Dispensed 0.000024 mL of Base (0.5 M KOH)
[44:27] Stepping pH = 7.21

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06007**
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Experiment start time: **3/6/2018 3:40:58 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[44:27] Dispensed 0.000024 mL of Base (0.5 M KOH)
[44:32] Stepping pH = 7.36
[44:47] Stirrer speed set to 0
[45:47] Datapoint id 45 collected
[45:47] Charge balance equation is out by -160.1%
[45:47] Stirrer speed set to 55
[45:52] pH 7.07 -> 7.27
[45:52] Using cautious pH adjust
[45:52] Dispensed 0.000024 mL of Base (0.5 M KOH)
[45:57] Stepping pH = 7.02
[45:57] Dispensed 0.000071 mL of Base (0.5 M KOH)
[46:02] Stepping pH = 7.98
[46:17] Stirrer speed set to 0
[47:17] Datapoint id 46 collected
[47:17] Charge balance equation is out by -347.1%
[47:17] Stirrer speed set to 55
[47:23] pH 8.04 -> 8.24
[47:23] Using cautious pH adjust
[47:23] Dispensed 0.000024 mL of Base (0.5 M KOH)
[47:28] Stepping pH = 8.03
[47:28] Dispensed 0.000024 mL of Base (0.5 M KOH)
[47:33] Stepping pH = 8.16
[47:33] Dispensed 0.000024 mL of Base (0.5 M KOH)
[47:38] Stepping pH = 8.35
[47:53] Stirrer speed set to 0
[48:53] Datapoint id 47 collected
[48:53] Charge balance equation is out by -699.5%
[48:53] Stirrer speed set to 55
[48:58] pH 8.43 -> 8.63
[48:58] Using cautious pH adjust
[48:58] Dispensed 0.000024 mL of Base (0.5 M KOH)
[49:03] Stepping pH = 8.46
[49:03] Dispensed 0.000024 mL of Base (0.5 M KOH)
[49:08] Stepping pH = 8.57
[49:09] Dispensed 0.000024 mL of Base (0.5 M KOH)
[49:14] Stepping pH = 8.69
[49:29] Stirrer speed set to 0
[50:12] Datapoint id 48 collected
[50:12] Charge balance equation is out by -340.0%
[50:12] Stirrer speed set to 55
[50:17] pH 8.69 -> 8.89
[50:17] Using cautious pH adjust
[50:17] Dispensed 0.000024 mL of Base (0.5 M KOH)
[50:22] Stepping pH = 8.69
[50:22] Dispensed 0.000024 mL of Base (0.5 M KOH)
[50:27] Stepping pH = 8.77
[50:27] Dispensed 0.000024 mL of Base (0.5 M KOH)
[50:32] Stepping pH = 8.86
[50:32] Dispensed 0.000024 mL of Base (0.5 M KOH)
[50:38] Stepping pH = 8.93
[50:53] Stirrer speed set to 0
[51:25] Datapoint id 49 collected
[51:25] Charge balance equation is out by -371.7%
[51:25] Stirrer speed set to 55
[51:30] pH 8.95 -> 9.05
[51:30] Using cautious pH adjust
[51:30] Dispensed 0.000024 mL of Base (0.5 M KOH)
[51:35] Stepping pH = 8.95
[51:35] Dispensed 0.000024 mL of Base (0.5 M KOH)

Sample name: **M09_octanol** Experiment start time: **3/6/2018 3:40:58 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-06007** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[51:40] Stepping pH = 8.96
[51:40] Dispensed 0.000071 mL of Base (0.5 M KOH)
[51:45] Stepping pH = 9.13
[52:00] Stirrer speed set to 0
[52:28] Datapoint id 50 collected
[52:28] Charge balance equation is out by -530.3%
[52:28] Titration 3 of 3
[52:28] Adding initial titrants
[52:28] Automatically add 0.10000 mL of Octanol
[52:30] Dispensed 0.100000 mL of Octanol
[52:30] Stirrer speed set to 10
[52:31] Stirrer speed set to 60
[52:31] Iterative adjust 9.13 -> 2.00
[52:31] pH 9.13 -> 2.00
[52:33] Dispensed 0.057314 mL of Acid (0.5 M HCl)
[52:38] pH 2.03 -> 2.00
[52:38] Dispensed 0.003387 mL of Acid (0.5 M HCl)
[53:28] Stirrer speed set to 0
[53:39] Datapoint id 51 collected
[53:39] Stirrer speed set to 60
[53:44] pH 1.97 -> 2.17
[53:44] Using cautious pH adjust
[53:44] Dispensed 0.009901 mL of Base (0.5 M KOH)
[53:49] Stepping pH = 2.06
[53:49] Dispensed 0.006914 mL of Base (0.5 M KOH)
[53:54] Stepping pH = 2.14
[53:55] Dispensed 0.001693 mL of Base (0.5 M KOH)
[54:00] Stepping pH = 2.17
[54:15] Stirrer speed set to 0
[54:25] Datapoint id 52 collected
[54:25] Charge balance equation is out by 6.5%
[54:25] Stirrer speed set to 60
[54:30] pH 2.17 -> 2.37
[54:30] Using charge balance adjust
[54:30] Dispensed 0.012535 mL of Base (0.5 M KOH)
[54:50] Stirrer speed set to 0
[55:00] Datapoint id 53 collected
[55:00] Charge balance equation is out by 6.7%
[55:00] Stirrer speed set to 60
[55:06] pH 2.38 -> 2.58
[55:06] Using charge balance adjust
[55:06] Dispensed 0.007808 mL of Base (0.5 M KOH)
[55:26] Stirrer speed set to 0
[55:36] Datapoint id 54 collected
[55:36] Charge balance equation is out by 10.7%
[55:36] Stirrer speed set to 60
[55:41] pH 2.61 -> 2.81
[55:41] Using charge balance adjust
[55:41] Dispensed 0.005009 mL of Base (0.5 M KOH)
[56:02] Stirrer speed set to 0
[56:12] Datapoint id 55 collected
[56:12] Charge balance equation is out by 2.5%
[56:12] Stirrer speed set to 60
[56:17] pH 2.82 -> 3.02
[56:17] Using charge balance adjust
[56:17] Dispensed 0.003551 mL of Base (0.5 M KOH)
[56:37] Stirrer speed set to 0
[56:47] Datapoint id 56 collected
[56:47] Charge balance equation is out by 13.2%

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
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Experiment start time: **3/6/2018 3:40:58 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[56:47] Stirrer speed set to 60
[56:52] pH 3.05 -> 3.25
[56:52] Using charge balance adjust
[56:52] Dispensed 0.002634 mL of Base (0.5 M KOH)
[57:13] Stirrer speed set to 0
[57:23] Datapoint id 57 collected
[57:23] Charge balance equation is out by 1.0%
[57:23] Stirrer speed set to 60
[57:28] pH 3.25 -> 3.45
[57:28] Using charge balance adjust
[57:28] Dispensed 0.002164 mL of Base (0.5 M KOH)
[57:48] Stirrer speed set to 0
[57:58] Datapoint id 58 collected
[57:58] Charge balance equation is out by 5.5%
[57:58] Stirrer speed set to 60
[58:03] pH 3.46 -> 3.66
[58:03] Using charge balance adjust
[58:03] Dispensed 0.001764 mL of Base (0.5 M KOH)
[58:24] Stirrer speed set to 0
[58:34] Datapoint id 59 collected
[58:34] Charge balance equation is out by 13.2%
[58:34] Stirrer speed set to 60
[58:39] pH 3.69 -> 3.89
[58:39] Using charge balance adjust
[58:39] Dispensed 0.001364 mL of Base (0.5 M KOH)
[58:59] Stirrer speed set to 0
[59:24] Datapoint id 60 collected
[59:24] Charge balance equation is out by 0.3%
[59:24] Stirrer speed set to 60
[59:29] pH 3.90 -> 4.10
[59:29] Using charge balance adjust
[59:29] Dispensed 0.001011 mL of Base (0.5 M KOH)
[59:49] Stirrer speed set to 0
[59:59] Datapoint id 61 collected
[59:59] Charge balance equation is out by -14.0%
[59:59] Stirrer speed set to 60
[1:00:05] pH 4.08 -> 4.28
[1:00:05] Using charge balance adjust
[1:00:05] Dispensed 0.000776 mL of Base (0.5 M KOH)
[1:00:25] Stirrer speed set to 0
[1:00:35] Datapoint id 62 collected
[1:00:35] Charge balance equation is out by -23.3%
[1:00:35] Stirrer speed set to 60
[1:00:40] pH 4.24 -> 4.44
[1:00:40] Using cautious pH adjust
[1:00:41] Dispensed 0.000282 mL of Base (0.5 M KOH)
[1:00:46] Stepping pH = 4.28
[1:00:46] Dispensed 0.000447 mL of Base (0.5 M KOH)
[1:00:51] Stepping pH = 4.41
[1:00:51] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:00:56] Stepping pH = 4.42
[1:00:56] Dispensed 0.000165 mL of Base (0.5 M KOH)
[1:01:01] Stepping pH = 4.46
[1:01:16] Stirrer speed set to 0
[1:01:27] Datapoint id 63 collected
[1:01:27] Charge balance equation is out by -64.5%
[1:01:27] Stirrer speed set to 60
[1:01:32] pH 4.46 -> 4.66
[1:01:32] Using cautious pH adjust

Sample name: **M09_octanol**   Experiment start time: **3/6/2018 3:40:58 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-06007**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06007_M09_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[1:01:32] Dispensed 0.000188 mL of Base (0.5 M KOH)
[1:01:37] Stepping pH = 4.52
[1:01:37] Dispensed 0.000235 mL of Base (0.5 M KOH)
[1:01:42] Stepping pH = 4.62
[1:01:42] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:01:47] Stepping pH = 4.63
[1:01:47] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:01:53] Stepping pH = 4.66
[1:02:08] Stirrer speed set to 0
[1:02:18] Datapoint id 64 collected
[1:02:18] Charge balance equation is out by -59.0%
[1:02:18] Stirrer speed set to 60
[1:02:23] pH 4.67 -> 4.87
[1:02:23] Using cautious pH adjust
[1:02:23] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:02:28] Stepping pH = 4.71
[1:02:28] Dispensed 0.000188 mL of Base (0.5 M KOH)
[1:02:34] Stepping pH = 4.84
[1:02:34] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:02:39] Stepping pH = 4.85
[1:02:39] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:02:44] Stepping pH = 4.86
[1:02:59] Stirrer speed set to 0
[1:03:10] Datapoint id 65 collected
[1:03:10] Charge balance equation is out by -59.7%
[1:03:10] Stirrer speed set to 60
[1:03:15] pH 4.87 -> 5.07
[1:03:15] Using cautious pH adjust
[1:03:15] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:03:20] Stepping pH = 4.88
[1:03:20] Dispensed 0.000212 mL of Base (0.5 M KOH)
[1:03:25] Stepping pH = 5.12
[1:03:41] Stirrer speed set to 0
[1:03:57] Datapoint id 66 collected
[1:03:57] Charge balance equation is out by -86.7%
[1:03:57] Stirrer speed set to 60
[1:04:02] pH 5.14 -> 5.34
[1:04:02] Using cautious pH adjust
[1:04:02] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:04:07] Stepping pH = 5.15
[1:04:07] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:04:12] Stepping pH = 5.43
[1:04:27] Stirrer speed set to 0
[1:04:48] Datapoint id 67 collected
[1:04:48] Charge balance equation is out by -88.8%
[1:04:48] Stirrer speed set to 60
[1:04:53] pH 5.48 -> 5.68
[1:04:53] Using cautious pH adjust
[1:04:53] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:04:59] Stepping pH = 5.49
[1:04:59] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:05:04] Stepping pH = 5.73
[1:05:19] Stirrer speed set to 0
[1:05:57] Datapoint id 68 collected
[1:05:57] Charge balance equation is out by -92.7%
[1:05:57] Stirrer speed set to 60
[1:06:02] pH 5.81 -> 6.01
[1:06:02] Using cautious pH adjust
[1:06:02] Dispensed 0.000024 mL of Base (0.5 M KOH)

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
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Experiment start time: **3/6/2018 3:40:58 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:06:07] Stepping pH = 5.82
[1:06:08] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:06:13] Stepping pH = 6.20
[1:06:28] Stirrer speed set to 0
[1:07:18] Datapoint id 69 collected
[1:07:18] Charge balance equation is out by -91.3%
[1:07:18] Stirrer speed set to 60
[1:07:23] pH 6.15 -> 6.35
[1:07:23] Using cautious pH adjust
[1:07:23] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:07:29] Stepping pH = 6.11
[1:07:29] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:07:34] Stepping pH = 7.70
[1:07:49] Stirrer speed set to 0
[1:08:49] Datapoint id 70 collected
[1:08:49] Charge balance equation is out by -243.1%
[1:08:49] Stirrer speed set to 60
[1:08:54] pH 7.85 -> 8.05
[1:08:54] Using cautious pH adjust
[1:08:54] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:08:59] Stepping pH = 7.89
[1:08:59] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:09:04] Stepping pH = 7.95
[1:09:04] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:09:09] Stepping pH = 8.07
[1:09:24] Stirrer speed set to 0
[1:10:24] Datapoint id 71 collected
[1:10:24] Charge balance equation is out by -683.0%
[1:10:24] Stirrer speed set to 60
[1:10:30] pH 8.14 -> 8.34
[1:10:30] Using cautious pH adjust
[1:10:30] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:10:35] Stepping pH = 8.19
[1:10:35] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:10:40] Stepping pH = 8.32
[1:10:40] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:10:45] Stepping pH = 8.48
[1:11:00] Stirrer speed set to 0
[1:12:00] Datapoint id 72 collected
[1:12:00] Charge balance equation is out by -550.4%
[1:12:00] Stirrer speed set to 60
[1:12:05] pH 8.50 -> 8.70
[1:12:05] Using cautious pH adjust
[1:12:05] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:12:10] Stepping pH = 8.51
[1:12:10] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:12:15] Stepping pH = 8.60
[1:12:15] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:12:21] Stepping pH = 8.68
[1:12:21] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:12:26] Stepping pH = 8.77
[1:12:41] Stirrer speed set to 0
[1:13:09] Datapoint id 73 collected
[1:13:09] Charge balance equation is out by -398.4%
[1:13:09] Stirrer speed set to 60
[1:13:14] pH 8.76 -> 8.96
[1:13:14] Using cautious pH adjust
[1:13:14] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:13:19] Stepping pH = 8.75

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
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Experiment start time: **3/6/2018 3:40:58 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:13:19] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:13:24] Stepping pH = 8.87
[1:13:24] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:13:29] Stepping pH = 9.01
[1:13:45] Stirrer speed set to 0
[1:14:08] Datapoint id 74 collected
[1:14:08] Charge balance equation is out by -368.3%
[1:14:08] Argon flow rate set to 0
[1:14:11] Titrator arm moved over Titration position